SPECTROSCOPIC STUDIES OF HYDROGEN COMPLEXES IN DIAMOND

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Abstract

New experimental data will be presented on hydrogen related complexes observed in as grown and annealed single crystal CVD diamond. The data has been obtained using a variety of spectroscopic techniques, but particular emphasis will be focused on the results of Infrared Absorption and Electron Paramagnetic Resonance studies, and these results will be interpreted in terms of molecular models for interstitial and substitutional hydrogen complexes in diamond. It will be shown that much of the accepted wisdom about hydrogen incorporation in diamond must be questioned.

INTRODUCTION

Hydrogen is an important impurity in silicon and III–V compound semiconductors. Particular interest has been focused on hydrogen passivation of donors or acceptors, as well as unwanted deep recombination centres. There is an ever-growing body of evidence that under appropriate conditions significant amounts of hydrogen can be incorporated in synthetic diamond grown via high temperature and pressure (HTHP) synthesis and chemical vapour deposition (CVD). Hydrogen is also a common impurity in natural diamond. Clear evidence for H-related complexes in CVD diamond comes from the passivation of boron acceptors by in-diffused deuterium [1]. It is reasonable to assume that a detailed understanding of the incorporation and properties of hydrogen in diamond will be required to ensure that single crystal CVD diamond emerges as the pre-eminent electronic material for extreme applications. Furthermore, an understanding of hydrogen incorporation should be invaluable to those modeling and perfecting synthesis, and provide insight into how hydrogen related complexes in natural diamond have evolved.

INCORPORATION OF HYDROGEN IN CVD DIAMOND

Recently attention has been focused on the structure and properties of vacancy-hydrogen and vacancy-nitrogen-hydrogen complexes in diamond detected by Electron Paramagnetic Resonance (EPR) [2,3]. Both these complexes have only been observed in CVD diamond. Fuchs and co-workers [4] observed several new absorption features in single crystal CVD diamond in the mid and near infrared spectral regions. Isotopic substitution has shown that several of these are hydrogen related, and recent work indicates that at high temperatures hydrogen is mobile in the diamond lattice and new hydrogen related complexes can be formed [5].

We will report the results of infrared absorption and EPR studies of hydrogen complexes in as grown and annealed single crystal CVD diamond. One of the defects studied in this way is the hydrogen vacancy complex, which has been shown to anneal out with an activation energy of 4.3(2) eV, which is comparable to the energy required to break a C-H bond. The consequences of this result for the diffusion of hydrogen in diamond will be discussed.

In addition to the quantitative EPR and infrared absorption measurements we have used uniaxial stress to probe the symmetry and electronic structure of hydrogen related complexes which have either or both vibrational and electronic optical absorption bands. Particular attention will be focused on the hydrogen related 3107 cm^{-1} infrared absorption band commonly detected in natural, and annealed synthetic diamond. A new model for this centre will be

presented. This assignment questions much of the accepted wisdom for hydrogen incorporation in diamond and the consequences of this identification will be discussed.

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